

National Ultrahigh-Field NMR Facility for Solids Centre national de RMN à ultrahaut champ pour les solides

Canadian NMR Research News Bulletin #7.1 Winter 2013



96th Canadian Chemistry Conference and Exhibition **QUÉBEC, QUEBEC** May 26-30, 2013 Chemistry Without Borders

Welcome Message

On behalf of the Organizing Committee of the **96th Canadian Chemistry Conference**, we are pleased to welcome you to Québec City from May 26 to 30, 2013. We hope that the scientific meetings set to take place in this cradle of Francophone culture in North America will be most fruitful.

The numerous fields discussed around the theme of *Chemistry Without Borders* will demonstrate the interdisciplinary nature of chemistry today.

CSC 2013 abstract submission deadline is **February 15, 2013** <u>http://www.csc2013.ca</u>

The conference will take place at the Centre des congrès de Québec located on Parliament Hill just steps from the Old City. Given its long tradition of hospitality, this city built "where the river narrows" will provide a most opportune setting for meeting by scientists from a broad range of horizons, both disciplinary and geographic. Québec City and its old European character will charm you, and its bars, enlivened by the songs of their numerous chansonniers, will be the scene of many a discussion without borders.

See you soon!

Mario Leclerc, Conference Co-Chair Armand Soldera, Conference Co-Chair Thierry Ollevier, Scientific Program Chair

CSC 2013 will feature several symposia with strong NMR content, including

Solid-state NMR Spectroscopy (PT – joint with BM)

<u>Organizers:</u> Michèle Auger (Laval), David Bryce (Ottawa)

<u>Invited Speakers:</u> Tatyana Polenova (Delaware), Ayyalusamy Ramamoorthy

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(Michigan), Luis Smith (Clark University, USA), Simon Sharpe (Toronto), Isabelle Marcotte (Université du Québec à Montréal), Suzana Straus (University of British Columbia), Peter Macdonald (Toronto), Rod Wasylishen (Alberta), Joe Zwanziger (Dalhousie), Kristopher Ooms (King's University College), Carl Michal (University of British Columbia).

Halogen Bonding and Other Non-Covalent Interactions (PT – joint with OR)

<u>Organizers:</u> David Bryce (Ottawa), Mark Taylor (Toronto)

Invited Speakers: Tim Bender (Toronto), Duncan Bruce (University of York, UK), Gino DiLabio (NRC-NINT), P. Shing Ho (Colorado State University), Tony Legon (University of Bristol, UK), Pierangelo Metrangolo (University of Milan, Italy), William Pennington (Clemson University, USA), Giuseppe Resnati (University of Milan, Italy), James Wuest (Université de Montréal).

8th Solid-State NMR Workshop brought to you by the National Ultrahigh-Field NMR Facility for Solids and Bruker Canada will take place Sunday, May 26, 2013, 13:00 - 19:00



Dear quest speakers, sponsors and attendees,

I would like to thank you all for your participation in our 5th Annual Symposium in November which was a great success again this year with officially 211 participants.

I would like more particularly to thank once again our quest speakers for having accepted our invitation, all of our poster presenters and, of course, our sponsors and exhibitors for their invaluable support.

I would like to congratulate again the graduate students and postdocs selected to give an oral presentation. Each of them received a nice certificate and \$150.

I would like also to congratulate the winners of our door prize drawing: Vanessa Mongeon (Second cup gift card - Corning), Juliana Munoz (Tim Hortons gift card - Fisher), Robert Harkness (Tim Hortons gift card -Fisher), **Pamela Zhang** (New England Biolabs gift bag), Irene Xie (Bruker gift package), Christine Hantouche (Bose head set - Agilent Technologies) and Asparouh Lilov (Boombox - GE Healthcare).

Please mark your calendar: the 6th Annual GRASP Symposium will be held on Monday, November 25th, 2013. We will look forward to seeing you all again next year.

Kind regards,

Annick

Annick Guyot, PhD **GRASP** Coordinator McGill University Bellini Bldg, Room 453 3649 Promenade Sir William Osler Montreal - QC - Canada - H3G 0B1

Phone: (+1) 514-398-2293 or (+1) 514-398-4323 extension 1 Fax: (+1) 514-398-2983 Email: grasp.med@mcgill.ca Web: http://grasp.mcgill.ca

New Funding announcements

2013 CFI Leading Edge Fund (LEF) and New Initiatives Fund (NIF)

In January 2013 the Government of Canada announced an investment of over \$215 million to support 75 projects at 34 institutions across the country through the Canada's Foundation for Innovation (CFI) Leading Edge Fund (LEF) and New Initiatives Fund (NIF), including

Structural biology at the crossroads of biology and medicine - project led by Prof. Kalle Gehring (McGill University, Department of Biochemistry, Faculty of Medicine) -\$4,834,800 – a joint project with Université de Montréal.

The grant will give researchers an improved ability to visualize the three-dimensional shapes of biological molecules, such as proteins and nucleic acids. This should lead to a better understanding of the origins of diseases such as cancer and to the design of novel molecules for use in structure-based drug design and green chemistry.

http://www.mcgill.ca/channels/news/investing-future-219797

Sustainable Chemical Synthesis from Renewable Feedstocks - project led by Prof. R. Tom Baker (University of Ottawa, Faculty of Science, Department of Chemistry and Canada Research Chair in Catalysis Science for Energy Applications) - \$5,732,853

As readily accessible fossil fuel resources decline, we are at a crossroads where petroleum refineries must make way for biorefineries: integrated systems that harness renewable biomass such as agricultural and wood wastes. This funding will enable the Centre for Catalysis Research and Innovation to explore the conversion of renewable biomass into fuel to significantly improve both the quality of our environment and Canada's competitiveness in clean energy technology.

http://www.media.uottawa.ca/mediaroom/news-details 2733.html

'How NMR Works' Informative Poster for Teaching Labs



Courtesy of the **SPINSIGHTS** team (Agilent Technologies, Inc.), NMR labs at universities and other settings that frequently train new users may find this informative graphic useful as a poster or handout.

To download a high-resolution PDF version: http://www.spinsights.net/

chemistry vitters | Your Information Nucleus A blog from the Chemical Institute of Canada

Posted on January 3, 2013 by Jodi Di Menna

Welcome to ChemistryMatters.ca!

Welcome to **ChemistryMatters.ca**, the blog of the Chemical Institute of Canada and its three Constituent Societies: the Canadian Society for Chemistry, the Canadian Society for Chemical Engineering and the Canadian Society for Chemical Technology.

We launched this blog in January 2013 to provide a place to provide thoughtful, timely and scientifically informed coverage of matters pertaining to the chemical sciences and engineering: new discoveries, industrial innovations, evolving policy and public understanding. Our goal is to provide the ultimate forum to exchange thoughts and ideas about where, how and why chemistry matters to us all.

To see the most recent posts and to find more about us visit

http://www.ChemistryMatters.ca

H.L. Holmes Award 2013: call for applications

The H.L. Holmes Award has been established by the National Research Council of Canada (NRC) in honour of the late Dr. R.H.L. Holmes, a chemist who spent most of his research career in Alberta.

Bequeathed by the late Dr. Holmes, in recognition of NRC's commitment to promote research excellence, the award gives recipients the opportunity to conduct post-doctoral studies under outstanding researchers at world famous graduate schools or research institutes. Research must be undertaken in chemistry, physics, biology or mathematics as they relate to medical and biological processes.

Awards cover a one or two-year period, depending on available funding and the research proposal, and can have a monetary value of up to \$100,000 CDN per year. Please consult the following link for more information:

http://www.nrc-cnrc.gc.ca/eng/outreach/holmes/index.html

Application Deadline: February 28, 2013

Call for Nominations: 2013 EAS New Faculty Award in NMR Spectroscopy

The Eastern Analytical invites nominations for an EAS New Faculty Award in NMR Spectroscopy. The Award will be presented at the 2013 Eastern Analytical Symposium, November 18-20, 2013, Somerset, NJ. The Award, sponsored by Agilent Technologies, **Inc.**, recognizes outstanding contributions by new faculty to the development of the field of NMR spectroscopy (broadly defined). To qualify for the award, candidates must at the time of the award hold a position as a tenure-track Assistant Professor in an academic institution in the US or Canada and be within 10 years of completing their terminal research degree. An Award winner will receive a certificate as well as \$2,000 and will deliver an award lecture at a dedicated EAS session.

Persons who wish to make a nomination for the EAS New Faculty Award in NMR Spectroscopy should send complete documentation of the candidate (nominating letter summarizing achievements, curriculum vita or resume, a statement of the nominee's willingness to present an address as part of the award symposium, and at least one seconding letter). The length of the nomination packet should be commensurate with the nominee's accomplishments, but should be limited to ten to fifteen pages. The deadline for the 2013 Award is **May 1, 2013**. The Awardee will be selected by the EAS NMR Awards Committee and notified by July 1, 2013.

Please send the nomination materials electronically (single PDF file is preferred) to: <u>awards@eas.org</u>

Tatyana Polenova, 2013 Awards Chair Eastern Analytical Symposium Visit us at: <u>http://eas.org</u>

NMR Theses Recently Defended

Marc-Olivier Séguin-Heine (Université du Québec à Montréal)

Supervisor: Prof. Isabelle Marcotte

M.Sc. thesis: "Étude de la teneur en métau, des propriétés mécaniques, de la structure et de la dynamique moléculaires des fibres de byssus de la moule en relation avec son environnement"

Monika M.M. Haring (University of Western Ontario) December 2012

Supervisor: Prof. Roberta Flemming

M.Sc. Geology: "Crystal structure and Al/Si cation ordering in "fassaite": A combined single crystal, ²⁷Al and ²⁹Si NMR Study". http://ir.lib.uwo.ca/etd/1058/

Margaret Hanson (University of Western Ontario) December 2012

Supervisors: Prof. Kim M. Baines and Prof. Yining Huang

Ph.D. Chemistry: "Structural Insights into Group 14 Compounds from Solid-State NMR Spectroscopy".

http://ir.lib.uwo.ca/etd/1032/

On the move

Fu Chen (Ph.D. 2009, Wasylishen group, Alberta) has accepted an Assistant Research Scientist position at the **University of Iowa** in the NMR facility centre. <u>http://chem.uiowa.edu/research/resources/nmr-facility</u>

Patrick Szell and **Julia Meyer** have joined the Bryce Group (University of Ottawa) as undergraduate researchers.

Recognition

Canadian Journal of Chemistry welcomes new Senior Editor

Reposted from http://www.nrcresearchpress.com/

NRC Research Press is pleased to welcome Professor **Yining Huang** of the Department of Chemistry at the University of Western Ontario as the new Senior Editor of the *Canadian Journal of Chemistry*. Professor Huang's appointment took effect January 1, 2013.



Yining earned his Ph.D. in Chemistry at McGill University and was a Natural Sciences and Engineering Research Council of Canada Postdoctoral Fellow at the University of British Columbia. He came to Western in 1997 and was Canada Research Chair in Materials Characterization from 2002 to 2012. He teaches in the areas of spectroscopy, inorganic, and materials chemistry. Yining's research is directed towards various porous materials, including zeolites, AIPO₄-based molecular sieves, metal-organic frameworks, and mesoporous materials, as well as various layered materials.

In addition to receiving many awards and honours, Professor Huang has been a prolific author, publishing in prominent chemistry journals around the world, including the *Canadian Journal of Chemistry*, where he was Materials Chemistry Editor from 2006 to 2012.

Professor Huang replaces outgoing Senior Editor, **Rob Lipson**, who has faithfully and tirelessly led the Journal for the past seven years. Many thanks to Rob for his service to the Journal and the chemistry community, and welcome aboard, Yining!

Learn more about the Canadian Journal of Chemistry

http://www.nrcresearchpress.com/journal/cjc

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NMR Events

54th ENC

April 14-19, 2013, Asilomar, CA http://www.enc-conference.org/



Surface Canada 2013 Conference: Energy, Materials, Environment

May 7-10, 2013, London, Ontario, Canada. http://sc2013.uwo.ca/

18th Triennial ISMAR Conference

May 19-24, 2013, Rio de Janeiro, Brazil http://www.ismar2013.net/



8th Solid-State NMR Workshop at CSC 2013

May 26, 2013, Québec, QC, Canada <u>http://nmr900.ca/events_e.html</u>

CSC 2013, the 96th Canadian Chemistry Conference and Exhibition "Chemistry without Borders"

May 26-30, 2013, Québec, QC, Canada http://www.csc2013.ca/

Computational Aspects of Metabolomic NMR Gordon Research Seminar

June 1-2, 2013, West Dover, VT

http://www.grc.org/programs.aspx?year=2013&program=grs_bionmr

Computational Aspects - Biomolecular NMR Gordon Research Conference

June 2-7, 2013 West Dover, VT http://www.grc.org/programs.aspx?year=2013&program=bionmr

7th Annual VIVA NMR Symposium

June, 2013, University of Victoria, Victoria B.C.

59th ICASS International Conference on Analytical Sciences and Spectroscopy & **Spectr'Atom 2013** Conference (June 25-28, 2013)

June 26-28, 2013, Le Grand Lodge Mont Tremblant, Mont-Tremblant, Québec <u>http://csass.org/ICASS.html</u> **EUROMAR 2013,** 30 June - 5 July, 2013, Hersonissos, Crete, Greece <u>http://www.euromar2013.org/</u>

NMRCM 2013 International Symposium and Summer School "NMR in Condensed Matter" 10th meeting "NMR in Life Sciences"

July 8-12, 2013, St. Petersburg, Russia http://nmr.phys.spbu.ru/nmrcm

55th Rocky Mountain Conference on Magnetic Resonance (EPR Symposium)

July 28-August 1, 2013, Denver, Colorado http://www.rockychem.com/

8th Alpine Conference on Solid-State NMR

September 8-12, 2013, Chamonix Mont-Blanc, France http://www.alpine-conference.org

SMASH 2013 Small Molecule NMR Conference

Sept 22-25, 2013, Santiago de Compostela, Spain <u>http://www.smashnmr.org/</u>

5th Asia-Pacific NMR Symposium (**APNMR5**) and 9th Australian & New Zealand Society for Magnetic Resonance (**ANZMAG**) Meeting

October 27-30, 2013, Brisbane, Australia http://apnmr2013.org/



November 25, 2013, McGill University, Montréal, QC, Canada http://grasp.mcgill.ca/english/conferences/conferences.html

CSC 2014, the 97th Canadian Chemistry Conference and Exhibition "Chemistry from Sea to Sky"

June 1-5, 2014, Vancouver, B.C., Canada

Pacifichem 2015 The International Chemical Congress of Pacific Basin Societies

December 15-20, 2015, Honolulu, Hawaii, USA http://www.pacifichem.org/

New NMR Books



NMR metabolomics in cancer research

Miroslava Cuperlovic-Culf (Author)

Hardcover: 446 pages Language: English Publisher: Woodhead Publishing, Jan 2013 ISBN: 978-1907568848

http://www.amazon.com/dp/1907568840 http://www.amazon.ca/dp/1907568840

About the Author

Dr. **Miroslava Cuperlovic Culf** is Research Officer at the National Research Council of Canada Institute for Information Technology (Moncton), Adjunct Professor of Chemistry at Mount Allison University and Adjunct Researcher at the Atlantic Cancer Research Institute. She has a range of publications and patents resulting from research in NMR spectral analysis and modeling, bioinformatics data analysis and computational biology for cellular pathway modeling, as applied to cancer research.

About the Book

- focused description of NMR spectroscopy needed by cancer biologists who are starting to use metabolomics

- current overview of knowledge related to the cancer metabolic phenotype from the perspective of metabolomics applications

- information about the best practices in NMR metabolomics experimentation and data preprocessing as applied to different sample types

- detailed description of various aspects of data analysis with examples from applications of NMR metabolomics including direct data analysis (unsupervised and supervised) as well as the use of metabolomics data (fluxomics) in metabolic pathway's model development

NMR metabolomics in cancer research presents a detailed account of the NMR spectroscopy methods applied to metabolomics mixture analysis along with a discussion of their advantages and disadvantages.

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http://www.woodheadpublishing.com/en/book.aspx?bookID=2827

eMagRes The Ultimate Online Resource for NMR and MRI

Wiley: eMagRes the Ultimate Online Resource for NMR and MRI

eMagRes captures every aspect of the interdisciplinary nature of magnetic resonance and provides the most complete and up-to-date online reference resource in the field. Currently **eMagRes** has published over 1,100 articles written by more than 1,250 experts.

eMagRes, previously published as Encyclopedia of Magnetic Resonance (EMR), presents the content in two ways. Firstly, the articles are organised alphabetically by topic, under the top-level headings of **MRI** and **NMR**. Secondly, articles are arranged chronologically: from 2012 onwards in **Volumes and Issues**, and prior to 2012 in annual supplements.

eMagRes is edited by leaders in the field, ensuring high quality, relevance, and topicality. For more information on the editorial team and contributors

http://onlinelibrary.wiley.com/book/10.1002/9780470034590/homepage/EditorsContributors.html

Since the original print publication of *Encyclopedia of Nuclear Magnetic Resonance* in 1996, the area of magnetic resonance has seen extensive developments and now encompasses a whole range of techniques, including MRI, MRS, NMR and ESR. *eMagRes* covers all the essential information on the science, methodologies, engineering, technologies, applications and the history of magnetic resonance. The quarterly addition of new articles and updates of existing articles ensures that *eMagRes* remains the most comprehensive, up-to-date reference in the field.

The articles on the history of NMR and MRI span the development of magnetic resonance from the 1940's to the latest developments. These "historical" articles add a very personal touch to the factual articles and make **eMagRes** a useful resource far beyond the interests of NMR and MRI specialists.

eMagRes is also the source of a unique series of print and e-books, containing articles carefully selected and commissioned for more focussed, specific readerships within the MRI and NMR communities.



For further information see

http://onlinelibrary.wiley.com/book/10.1002/9780470034590

NMR Software

EZNMR at the University of Ottawa

Glenn Facey

gafacey@uottawa.ca

The NMR Facility at the University of Ottawa is equipped with eight NMR spectrometers and has on the order of 100 hands-on users at the graduate and post-doctoral level. Like any university NMR facility, the users enter at varving knowledge and experience levels: from "What does NMR stand for?" to "How do I do a shearing transform for my 50MAS data set?". Also, the attitude of the user's supervisors varies considerably. Some supervisors want their students to spend as little time in the NMR lab as possible by collecting all of their data in automation with a sample changer so they can maximize their time at the bench. Others want their students to learn how to collect the best possible data and fully understand the NMR measurements they make. There is no doubt that collecting NMR data under complete automation is incredibly time-efficient however, collecting data in this way teaches the student nothing about NMR measurements. On the other hand, learning to use NMR spectrometers manually, at the most fundamental level, to collect the best possible data, requires a great deal of knowledge (both general and instrument-specific) and although it is the most educationally rewarding, it certainly provides less overall sample throughput. In our facility, almost all students are first given 10 minutes of training, on how to collect NMR data under complete automation using our only fully automated instrument. Running an NMR spectrometer in this way requires absolutely no knowledge of NMR spectroscopy. Most users are also interested in using the other less automated instruments. These students are provided with as much training as they desire. The job of the NMR facility is to educate and satisfy the needs or each user. Doing so, requires finding a "happy medium" between complete automation and complete manual spectrometer operation and using that medium as a minimum training standard. For the last ten years or so, the "happy medium" used by the University of Ottawa to run four of it its Bruker NMR instruments is based on a customized button panel approach. We have written button panels specific to each instrument and call the

option **EZNMR**. We have included **EZNMR** as an entry on the top TOPSPIN menu bar. Clicking the **EZNMR** option opens up a button panel like the one shown below, used on our AVANCE 500 spectrometer.



Each button either issues a command, runs a macro or runs an "au program". Some of our students use exclusively this panel to collect their data. The advantage to using such a system is that the student must at least learn all of the steps involved with collecting the data. A typical **EZNMR** session involves simply following the button panel from top to bottom. If the probe contains a sample, it is ejected with the **EJECT** button. A new sample is

lowered into the probe with the **INSERT** button. The deuterium lock is established by pressing the LOCK button which prompts the user for the solvent and then establishes the lock. The SHIM button first calls up a standard set of shims and then initiates a gradient shimming routine. After the magnet is shimmed, the user presses any one of the green buttons depending on which NMR measurement they intend to carry out. Pressing one of these buttons prompts the user to define a data set and then calls up a reasonable set of parameters into that data set. If desired, the user can change the number of scans or some of the parameters by pressing the SCANS or PARAMETERS buttons. The probe is then tuned using the **TUNE** button. The **START** button optimizes the receiver gain and begins collecting the data. Once started, the data can be processed at any time using the **Proc 1D** button or halted using the HALT button. We use a similar button panel for the commonly used 2D NMR experiments which can be called up from the 1D panel. It is shown here:



The advantages to using this system are:

- It is highly customizable for the hardware of each instrument as it is based on macros and "au programs".

- It can be added to as demands change.

- All NMR spectrometers using EZNMR look pretty much the same so instrument specific training is less of an issue.

- Students can begin running NMR experiments very quickly.

- Students are more likely to ask questions about each step and can learn at their own pace while maintaining high sample throughput.

- Its use is entirely optional.

- It is much more time-efficient than complete manual operation.

Feel free to contact me via email if you would like a copy of the code.

Glenn

Dr. Glenn A. Facey NMR Facility Manager

Department of Chemistry University of Ottawa 10 Marie Curie, Ottawa, Ontario K1N 6N5 CANADA

ph. (613) 562-5800 ext 6077 fax. (613) 562-5170 email: gafacey@uottawa.ca

web: <u>http://www.science.uottawa.ca/nmr</u> http://www.u-of-o-nmr-facility.blogspot.com

contributed by David Bryce (Ottawa)

QUEST – QUadrupolar Exact SofTware

QUEST is a new program for the exact simulation of solid-state NMR spectra of quadrupolar nuclei in stationary powdered samples which employs diagonalization of



the combined Zeeman-guadrupolar Hamiltonian. The program may be used to simulate NMR spectra over the full regime of Larmor and quadrupolar frequencies, which encompasses scenarios ranging from high-field NMR to nuclear quadrupole resonance (NQR, where the Larmor frequency is zero) and does not make use of approximations when treating the guadrupolar interaction. The program, which uses a graphical user interface, also incorporates chemical shift anisotropy and non-coincident chemical shift and quadrupolar tensor frames. QUEST can be used to simulate static NMR and NOR spectra with any relative size of the Zeeman and quadrupolar interactions and correctly predicts the appearance of "forbidden" or "overtone" NMR as well as NQR transitions.

The most recent version of **QUEST** is available from the software link on our webpage <u>http://mysite.science.uottawa.ca/dbryce/</u>

NMR Jobs and Vacancies

M.Sc. or Ph.D. position in solid-state NMR at the University of Ottawa

Highly motivated candidates interested in physical chemistry and/or NMR spectroscopy are invited to apply for a M.Sc. or Ph.D. in the group of **Prof. David Bryce** at the University of Ottawa

http://mysite.science.uottawa.ca/dbryce/

Research in solid-state NMR in the Bryce group covers a variety of areas including the development of the spectroscopy of traditionally difficult quadrupolar nuclei, applications of double-rotation NMR, applications to weak interactions including halogen bonding, and the study of polymorphism. Experimental work is complemented by quantum chemical studies. Interested students should contact Prof. Bryce directly at <u>dbryce@uottawa.ca</u>

Please note that due to budgetary constraints, the position is open only to Canadian students.

Prof. David L. Bryce, Ph.D.

Department of Chemistry 10 Marie Curie Private University of Ottawa Ottawa, Ontario K1N6N5 Canada Phone 613-562-5800 ext 2018 Fax 613-562-5170 Email <u>dbryce@uottawa.ca</u> Web http://mysite.science.uottawa.ca/dbryce/

PhD/Post-doc positions in NMR characterization of transport in novel energy materials and devices

Institute for Frontier Materials, Deakin University, Waurn Ponds Campus, Geelong, Victoria, Australia <u>http://www.deakin.edu.au/research/ifm/index.php</u>

Selective transport of certain molecules or ions through a material or across a barrier is a phenomenon of critical importance to many physical, chemical and biological processes. For example technologies such as CO_2 capture and energy storage require selective transport of species such as CO_2 , Li⁺, Na⁺ or H⁺. Magnetic resonance offers unique tools capable of probing the environment and transport of these species via the observation of target nuclei. Techniques such as NMR spectroscopy, pulsed field gradient diffusion measurements and micro-imaging allow us to investigate transport within model materials or even fullscale devices such as batteries.

We are offering the opportunity to a chemist, physicist or materials scientist to undertake PhD study or post-doctoral research within the Institute for Frontier Materials at Deakin University (Victoria, Australia). This will involve the application of magnetic resonance techniques towards a better understanding of structure-property relationships in energy materials such as polymer electrolytes, ionic liquids, plastic crystals, and devices based on these (e.g. CO_2 membranes or metal-air batteries).

Successful candidates will work as part of a large inter-disciplinary team and will gain experience in a broad range of NMR methods, both in techniques development and applications to real, state-of-the-art material systems. Prior experience in magnetic resonance, ideally in micro-imaging or NMR methodological development, is mandatory for the post-doctoral position, and would be advantageous for the PhD candidate.

For more information on these positions please contact **Dr. Luke O'Dell** luke.odell@deakin.edu.au

or Prof. Maria Forsyth

maria.forsyth@deakin.edu.au

Luke O'Dell Senior Lecturer in NMR Spectroscopy Institute for Frontier Materials Deakin University Waurn Ponds Campus Geelong, Victoria 3220, Australia Office: 03 522 73076 http://www.deakin.edu.au/research/ifm/staff.php?contact_id=722

Postdoctoral NMR positions

Postdoctoral Position in enzymology, Iowa State University, Ames, Iowa http://nmr900.ca/nmr_jobs.html#iowa

Stanford University, Postdoctoral Position in Peptide/Protein NMR <u>http://nmr900.ca/nmr_jobs.html#stanford</u>

Canadian NMR Research Highlights

NMR papers in Angewandte Chemie

R. Evans, Z. Deng, A.K. Rogerson, A.S. McLachlan, J.J. Richards, M. Nilsson, G.A. Morris, "Quantitative Interpretation of Diffusion-Ordered NMR Spectra: Can We Rationalize Small Molecule Diffusion Coefficients?," Angewandte Chemie International Edition (2013) online. http://dx.doi.org/10.1002/anie.201207403

R. Kumar, D.D. Klug, C.I. Ratcliffe, C.A. Tulk, and J.A. Ripmeester, "Low-Pressure Synthesis and Characterization of Hydrogen-Filled Ice Ic," Angewandte Chemie International Edition 52 (2013) 1531–1534. http://dx.doi.org/10.1002/anie.201208367



Current Opinion in Chemical Biology

Mechanisms Edited by Stephen G. Withers (UBC) and David J. Vocadlo (SFU)

volume 16 (2012) issue 5-6

http://www.sciencedirect.com/science/iournal/13675931/16/5-6

D.J. Vocadlo, S.G. Withers, " Editorial overview: How to make a difference: mechanisms of protein and nucleic acid modifying enzymes," Current Opinion in Chemical Biology 16 (2012) 461-464. http://dx.doi.org/10.1016/j.cbpa.2012.10.033

A.J. Bennet, "Kinetic isotope effects for studying post-translational modifying enzymes," Current Opinion in Chemical Biology 16 (2012) 472-478. (Review) http://dx.doi.org/10.1016/j.cbpa.2012.10.024

Progress in NMR Spectroscopy



U.H.N. Dürr, R. Soong, A. **Ramamoorthy**, "When detergent meets bilayer: birth and coming of age of lipid bicelles," Progress in Nuclear Magnetic Resonance Spectroscopy (2013) online. (Invited Review) http://dx.doi.org/10.1016/j.pnmrs.2013.01.0

NMR papers in PNAS

A.M. Ruschak, L.E. Kay, "Proteasome allostery as a population shift between interchanging conformers," PNAS 109 (2012) E3454-E3462.

http://dx.doi.org/10.1073/pnas.1213640109

A. Sekhar, P. Vallurupalli, L.E. Kay, "Folding of the four-helix bundle FF domain from a compact on-pathway intermediate state is governed predominantly by water motion," PNAS 109 (2012) 19268-19273. http://dx.doi.org/10.1073/pnas.1212036109

Review in Natural Product Reports

R.C. Breton and W.F. Reynolds, "Using NMR to identify and characterize natural products." Natural Product Reports (2013) online. (Review) http://dx.doi.org/10.1039/C2NP20104F

Reviews in Solid State Nuclear Magnetic Resonance

F.A. Perras, J. Viger-Gravel, K.M.N. Burgess, D.L. Bryce, "Signal Enhancement in Solid-State NMR of Quadrupolar Nuclei," Solid State Nuclear Magnetic Resonance (2013) online. (Review) http://dx.doi.org/10.1016/j.ssnmr.2012.11.002

A. Sutrisno and Y. Huang, "Solid-state NMR: a Powerful tool for Characterization of Metalorganic Frameworks," Solid State Nuclear Magnetic Resonance **49-50** (2013) 1–11. (Invited Review)

http://dx.doi.org/10.1016/j.ssnmr.2012.09.003

Chemical Reviews

H.A. Taha, M.R. Richards, and T.L. Lowary, "Conformational Analysis of Furanoside-Containing Mono- and Oligosaccharides," Chemical Reviews (2013) online. (Review) http://dx.doi.org/10.1021/cr300249c

Reviews in Chemistry and Physics of Lipids

P.M. Macdonald, Q. Saleem, A. Lai, H.H. Morales, "NMR Methods for Measuring Lateral Diffusion in Membranes," Chemistry and Physics of Lipids 166 (2013) 31-44. (Review) http://dx.doi.org/10.1016/j.chemphyslip.2012.12.004

Recent NMR Publications

most recent NMR publications by Canadian research groups as they appear on <u>http://nmr900.ca</u> website. This list should not be considered complete. You are encouraged to let us know of your recent publications as they become available.

Memorial University of Newfoundland

Y. Zhao, T. Luu, G.M. Bernard, T. Taerum, R. McDonald, R.E. Wasylishen, R.R.

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Contact us

Victor Terskikh, Manager National Ultrahigh-field NMR Facility for Solids

1200 Montreal Road M-40 Ottawa ON, K1A 0R6 Tel. (613) 998-5552 Fax: (613) 990-1555

Email: terskikhv@nrc-cnrc.gc.ca